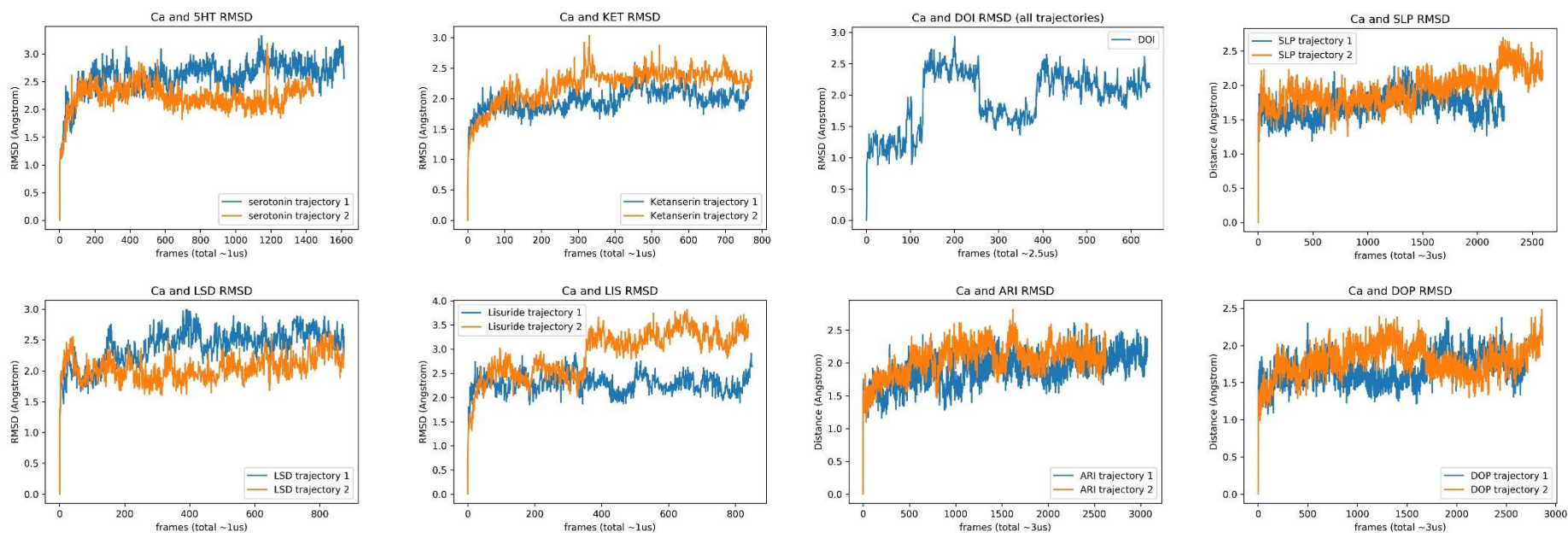


# A Machine Learning Approach for the Discovery of Ligand-specific Functional Mechanisms of GPCRs

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**Figure S1.** RMSD of the alpha carbon and ligand heavy atoms over the trajectories. The two trajectories of each ligand are colored in blue and orange, respectively, except for DOI for which 25 independently run trajectories are concatenated serially.